

# Magnetic properties of the Hubbard model on three-dimensional lattices: fluctuation-exchange and two-particle self-consistent studies

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The relation between three-dimensional lattice structure and magnetism in correlated electron systems is explored for face centered cubic (FCC), body centered cubic (BCC), and simple cubic (SC) lattices. In particular, we question which lattice structure has the strongest tendency toward the ferromagnetism or antiferromagnetism. We employ the Hubbard model to calculate the spin susceptibility and the single-particle spectrum with the fluctuation-exchange (FLEX) and the two-particle self-consistent (TPSC) approximations in the weak coupling regime. We have shown that (i) ferromagnetic spin fluctuations become dominant when the Fermi level lies around a sharp peak (divergence) in the density of states ( $D(E)$ ) near the bottom of the band, which occurs for FCC with/without next nearest neighbor hoppings ( $t'$ ) or BCC with an appropriate value of  $t'$ . Among the cases studied, the ferromagnetic fluctuation is found to be the strongest for FCC with a finite  $t'$ . (ii) When the peak in  $D(E)$  resides around the band center as in bipartite SC or BCC, antiferromagnetic fluctuations become dominant when the band is close to the half-filling, with the fluctuation being much stronger in BCC.

**KEYWORDS:** three-dimensional Hubbard model, ferromagnetism, antiferromagnetism, fluctuation exchange approximation, two-particle self-consistent approximation

## §1. introduction

The metallic ferromagnetism in repulsively interacting electron systems is among central problems in solid state physics, but is still some way from a complete understanding despite a long history of investigations. After the seminal papers by Kanamori,<sup>1)</sup> by Hubbard,<sup>2)</sup> and by Gutzwiller<sup>3)</sup> appeared back in the 1960's, the single-band Hubbard model has been studied intensively to understand metallic ferromagnetism. Although it is a simplest one conceivable, the model can still harbor insights into the fundamental mechanism for an itinerant ferromagnetism in correlated electron systems.

Historically, a guiding principle for realizing ferromagnetic states was provided by Stoner's mean field theory, which suggests that the ferromagnetic state should be favored for large enough interaction and/or density of states (DOS) at the Fermi level. Kanamori<sup>1)</sup> elaborated this argument with the T-matrix approximation to show that the ferromagnetic states are indeed favored when a peak in the DOS around the Fermi level is embedded around the bottom of the wide band. However, for general band filling, the extent to which the T-matrix approximation is valid is not clear.

As a different avenue along this line, rigorous results were recently obtained for ferromagnetism on specific lattices having flat bands. Lieb<sup>4)</sup> has shown that, when we have a bipartite lattice with different numbers of sublattice sites, the ground state at half filling should be ferrimagnetic for arbitrary magnitudes of the repulsion,  $U$ . Different numbers of sublattice sites imply that there is a flat band(s) in the one-electron band structure, or a delta-function density of states. Mielke and Tasaki<sup>5)</sup>

then proved the existence of ferromagnetic ground states in systems with flat band for more general classes of lattices.

Going back to ordinary lattices, one can then look for divergences in the DOS to realize a ferromagnetic state in the Hubbard model. For three-dimensional lattices, the divergence occurs for the face centered cubic (FCC) lattice (where the DOS diverges at the band bottom, or above the bottom if we include next-nearest neighbor hopping,  $t'$ ) or for the body centered cubic (BCC) lattice (where the DOS diverges at the center due to the electron-hole symmetry, or away from the center if we include an appropriate value of  $t'$ ). Our question here is 'among the lattice structures having sharply peaked (divergent) DOS's which one has the strongest tendency toward ferromagnetism?'. While the fully polarized ground state is expected to be favored when the DOS diverges near the bottom of the band, the tendency toward the ferromagnetic instabilities at finite temperatures is a non-trivial problem, because  $T_C$  of a system whose ground state is fully polarized is not necessarily higher than that of a system whose ground state is partially polarized.

As the background for the problem we can first recapitulate how the link between the lattice structure and the ferromagnetism has been understood in terms of the Hubbard model.<sup>6)</sup> The link may be tested accurately in one-dimensional(1D) systems, since the density matrix renormalization group (DMRG) method developed by White<sup>7)</sup> is applicable in 1D. Recently, a saturated ferromagnetic ground state has been found in the Hubbard model on various lattices. These include a trestle chain<sup>8,9,10)</sup> which may be regarded as a generalized flat

band model in 1D,<sup>11)</sup> ladder systems<sup>12,13)</sup> and nearly flat-band models.<sup>14)</sup>

In the opposite limit of infinite dimensions, exact calculation by means of dynamical mean field theory (DMFT) becomes feasible, since the self energy becomes site-diagonal or  $\mathbf{k}$ -independent. Using finite-temperature quantum Monte Carlo (QMC) techniques, Ulmke<sup>15)</sup> has solved the DMFT equations to discuss the stability of metallic ferromagnetism for FCC-type lattices in infinite dimensions. Wegner *et al.*<sup>16)</sup> obtained similar results with an iterated perturbation theory instead of QMC. If one compares these results with that for the hypercubic lattice by Obermeier *et al.*,<sup>17)</sup> FCC is seen to be favorable for ferromagnetism.

For two-dimensional (2D) or three-dimensional (3D) systems, which are of realistic interests, the situation is less conclusive, since we cannot apply the  $d = \infty$  result straightforwardly. For 2D Hlubina *et al.*<sup>18,19)</sup> suggested a possibility of the ferromagnetic ground state when the Fermi level is located near the van Hove singularity in the  $t$ - $t'$  Hubbard model for low densities. For 3D there are many studies with a variety of approximate methods. Hanisch *et al.*<sup>20)</sup> studied the instability of Nagaoka's saturated ferromagnetic ground state<sup>21)</sup> for various lattices with a variational method. The DMFT, which has originally been developed for  $d = \infty$ , has also been applied to 3D by Ulmke<sup>15)</sup> by plugging the DOS of the FCC lattice into the DMFT equations to obtain the phase diagram for FCC. However, the validity of the approximation, i.e., whether we can neglect the  $\mathbf{k}$ -dependence of the self energy in 3D, is quite an open question. Nolting<sup>22)</sup> *et al.* also studied the stability of the ferromagnetic state for the FCC Hubbard model with the spectral density approach, which may give reasonable results in the strong coupling limit,<sup>23)</sup> but the obtained  $T_C$  turns out to be several times larger than those estimated in the DMFT.

Since the above approaches involve one approximation or another (such as the strong-coupling limit, infinite dimension, etc), further investigations with different approaches should shed a new light on the problem. The purpose of the present paper is to investigate the magnetic properties of the 3D Hubbard model from the weak-coupling side, where the fluctuation-exchange (FLEX) and the two-particle self-consistent (TPSC) approximations are used to explore ferromagnetism for the first time. With these methods we look into FCC, BCC, and simple cubic (SC) lattices with or without next-nearest neighbor hoppings.

The FLEX, introduced by Bickers *et al.*,<sup>26,27)</sup> takes a set of skeleton diagrams for Luttinger-Ward functional to generate a ( $k$ -dependent) self energy that is computed self-consistently based on the idea of Baym and Kadanoff.<sup>24,25)</sup> Hence the FLEX is a kind of self-consistent perturbation approximation with respect to  $U$ . The method has been applied to the analysis of the 2D Hubbard model<sup>26,27,28,29)</sup> in the context of high- $T_c$  cuprates, superconducting ladder systems<sup>30)</sup> or organic superconductors.<sup>31,32)</sup> The FLEX breaks down in the intermediate to strong coupling regimes where the vertex corrections become significant, as seen from the fact that the pseudo-gap or the Hubbard bands are not repro-

duced,<sup>33)</sup> but the method should give reasonable results at least in the weak-coupling regime, namely as far as the fluctuations do not grow too much.

In Kanamori's theory,<sup>1)</sup> vertex correction is taken into account with the T-matrix approximation, which is only valid in the dilute limit. Here we have opted for the FLEX approximation, since the theory, with no restrictions on the electron density, can discuss the density dependence of the spin fluctuation, although the vertex corrections are neglected with only the self-energy corrections are taken into account there. In this context, Moriya and Takahashi<sup>34)</sup> developed a theory which takes account of both the vertex corrections and the self-energy corrections. Along this line, Usami and Moriya<sup>35)</sup> discussed the ferromagnetic metals such as Fe, Co, Ni with a functional integral method. Similar or more elaborate calculations were done by Hasegawa<sup>36)</sup> and by Hubbard.<sup>37)</sup> However, these are done at the cost of introducing phenomenological parameters, while the FLEX can be implemented from a microscopic level (e.g., the Hubbard model) without introducing any phenomenological parameters.

The TPSC method, on the other hand, takes vertex correction into account in a self-consistent manner at the two-body level by assuming a parameterized form for the Luttinger-Ward functional, where renormalized interactions  $U_{\text{sp}}$  and  $U_{\text{ch}}$  are introduced. In term of these 'effective  $U$ ' we assume the same functional forms (see eqns (19,20) below) as in the RPA for charge/spin susceptibilities. These parameters are determined so as to satisfy the sum rules or the constraints on a two-particle property, e.g., the double occupancy  $\langle n_{\uparrow}n_{\downarrow} \rangle$ . For the 2D Hubbard model on square lattice, Vilk *et al.*<sup>33)</sup> succeeded in reproducing the pseudo-gap and the upper/lower Hubbard bands, which indicates that the TPSC approach may be valid in the intermediate coupling regime as well.<sup>38)</sup> However, a numerical difficulty can arise in the calculation of the chemical potential as we shall see later (§III A), so we concentrate on the FCC lattice with next-nearest neighbor hoppings, for which the ferromagnetic spin fluctuation turns out to be the strongest among the cases studied in FLEX, and is of interest.

Both FLEX and TPSC methods will become invalid in the strong-coupling regime, while strong repulsion is often thought to be required for the realization of ferromagnetic ground states as in Nagaoka's case.<sup>21)</sup> Nevertheless, we expect that the tendency toward a ferromagnetic phase transition in the weak-coupling approach may be captured even when the transition itself occurs outside the regime. Here we have numerically checked to which value of  $U$  the method may be relied upon. Another purpose of the present paper is to discuss in which lattice structure the *antiferromagnetism* is most favored. Antiferromagnetism, contrary to ferromagnetism, is tractable with approaches in the weak-coupling regime in general.

The present paper is then organized as follows. In section II, after introducing the model, we review the formalism of FLEX and TPSC. Section III is devoted to the results and discussions, while section IV summarizes the results.

## §2. Formulation

### 2.1 Model Hamiltonian

We consider the conventional single-band Hubbard model,

$$\mathcal{H} = \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where  $c_{i\sigma}^\dagger$  creates an electron at the  $i$ -th site with spin  $\sigma$ ,  $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$  is the number operator. We take  $t_{ij} = t$  for nearest neighbors and  $t_{ij} = t'$  for second-nearest neighbors. The energy dispersions for FCC, BCC, and SC lattices are given as

$$\varepsilon^{\text{FCC}}(\mathbf{k}) = 4t \sum_{i < j} \cos(k_i) \cos(k_j) + 2t' \sum_{i=1}^3 \cos(2k_i), \quad (2)$$

$$\varepsilon^{\text{BCC}}(\mathbf{k}) = 8t \cos(k_1) \cos(k_2) \cos(k_3) + 2t' \sum_{i=1}^3 \cos(2k_i) \quad (3)$$

$$\varepsilon^{\text{SC}}(\mathbf{k}) = 2t \sum_{i=1}^3 \cos(k_i), \quad (4)$$

respectively, where  $k_1 \equiv k_x$ ,  $k_2 \equiv k_y$ ,  $k_3 \equiv k_z$ . To facilitate the calculation here we take a cubic Brillouin zone ( $-\pi < k_i \leq \pi$ ) by considering two(four) equivalent, interpenetrating FCC(BCC) lattices. Hereafter, we set  $t = 1$ .

### 2.2 The FLEX approximation

We first review the formalism of the FLEX approximation. We start from the Luttinger-Ward functional  $\Phi$  which is defined as  $\Omega = \Phi + T \sum [\ln G - \Sigma G]$ , where  $\Omega$  is the thermodynamic potential,  $G$  is the dressed Green's function and  $\Sigma$  is the self energy. The Feynman diagrams for  $\Phi$  considered in the FLEX approximation are shown in Fig. 1.

Fig. 1. The Luttinger-Ward functional considered in the FLEX approximation. Full lines represent the dressed Green's function while broken lines  $U$ . The summation is over  $n$ , the total number of interaction lines.

The self energy can be obtained with a functional derivative as

$$\begin{aligned} \Sigma(k) &= \delta\Phi/\delta G \\ &= \frac{1}{N} \sum_q \left[ G(k-q) V^{(2)}(q) \right. \\ &\quad \left. + G(k-q) V^{(\text{ph})}(q) + G(-k+q) V^{(\text{pp})}(q) \right]. \end{aligned} \quad (5)$$

This consists of the contribution from the bubble diagrams,

$$V^{(2)}(q) = U^2 \chi_{\text{ph}}(q), \quad (6)$$

the contribution from the particle-hole channel,

$$V^{(\text{ph})}(q) = \frac{1}{2} U^2 \chi_{\text{ph}}(q) \left[ \frac{1}{1 + U \chi_{\text{ph}}(q)} - 1 \right]$$

$$+ \frac{3}{2} U^2 \chi_{\text{ph}}(q) \left[ \frac{1}{1 - U \chi_{\text{ph}}(q)} - 1 \right], \quad (7)$$

(8)

and the contribution from the particle-particle channel,

$$V^{(\text{pp})}(q) = -U^2 \chi_{\text{pp}}(q) \left[ \frac{1}{1 + U \chi_{\text{pp}}(q)} - 1 \right] \quad (9)$$

where

$$\chi_{\text{ph}}(q) = -\frac{1}{N} \sum_k G(k+q) G(k), \quad (10)$$

$$\chi_{\text{pp}}(q) = \frac{1}{N} \sum_k G(k+q) G(-k). \quad (11)$$

Here we have denoted  $q \equiv (\mathbf{q}, i\epsilon_\nu)$  and  $k \equiv (\mathbf{k}, i\omega_n)$ ,  $\epsilon_\nu = 2\pi\nu T$  is the Matsubara frequency for bosons while  $\omega_n = (2n-1)\pi T$  for fermions, and  $N$  is the total number of sites.

The Dyson equation is written as

$$G(\mathbf{k}, \omega_n)^{-1} = G^0(\mathbf{k}, \omega_n)^{-1} - \Sigma(\mathbf{k}, \omega_n), \quad (12)$$

where

$$G^0(\mathbf{k}, \omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}}^0}, \quad (13)$$

is the bare Green's function with  $\varepsilon_{\mathbf{k}}^0$  being the energy for the free electrons.

We solve the equations (5) ~ (12) by setting the chemical potential  $\mu$  so as to fix the density of electrons. The Green's function is computed by iteration until a convergence condition,

$$|G^{(r)}(k) - G^{(r-1)}(k)|/|G^{(r)}(k)| < 1.0 \times 10^{-4}, \quad (14)$$

for  $G^{(r)}(k)$ , the Green's function at the  $r$ -th iteration, is attained for all the values of  $k$ . We have checked the convergence by taking (i)  $16^3$  sites for which 1024 Matsubara frequencies ( $-1023\pi T \leq \epsilon_\nu \leq 1023\pi T$ ) or 2048 frequencies are considered, and (ii) a larger  $32^3$  sites with 1024 Matsubara frequencies.

We define the RPA spin susceptibility as

$$\chi_{\text{RPA}}(q) = \frac{\chi_{\text{ph}}(q)}{1 - U \chi_{\text{ph}}(q)}.$$

There is no vertex correction in this expression. As for the static magnetic susceptibility,  $\chi(0)$  can be calculated, as pointed out by McQueen *et al.*,<sup>39)</sup> from the slope  $\text{Tr}[\sigma_z G]$  versus small homogeneous field  $h$  (typically  $0.005t \sim 0.01t$ ), where  $\sigma_z$  is the  $z$ -component of the Pauli matrix. This is equivalent to solving an integral equation for the response function with irreducible vertices comprising particle-particle and particle-hole bubble chains along with the Aslamazov-Larkin type diagrams.

The integrated spectral function, or the DOS, is given by

$$\rho(\omega) = -\frac{1}{\pi} \sum_{\mathbf{k}} \text{Im} G(\mathbf{k}, \omega + i\delta).$$

We obtain  $G(\mathbf{k}, \omega)$  by a numerical analytic continuation from the imaginary-axis data,  $G(\mathbf{k}, i\omega_n)$ , with the Padé approximation.<sup>40)</sup>

### 2.3 The TPSC approximation

Next we review the TPSC method following the argument by Vilk and Tremblay.<sup>33)</sup> This method starts from assuming that the Luttinger-Ward functional  $\Phi$  can be parameterized by two variables,  $\Gamma_{\sigma-\sigma}$  and  $\Gamma_{\sigma\sigma}$ , as

$$\Phi = \frac{N}{2} \sum_{\sigma} \left[ \tilde{G}_{\sigma}(0^+) \Gamma_{\sigma\sigma} \tilde{G}_{\sigma}(0^+) + \tilde{G}_{\sigma}(0^+) \Gamma_{\sigma-\sigma} \tilde{G}_{-\sigma}(0^+) \right] \quad (15)$$

with

$$\tilde{G}_{\sigma}(0^+) = \frac{T}{N} \sum_k \exp(ik0^+) G_{\sigma}(k). \quad (16)$$

If we introduce spin and charge irreducible vertices as

$$U_{\text{sp}} \equiv \Gamma_{\sigma-\sigma} - \Gamma_{\sigma\sigma}, \quad (17)$$

$$U_{\text{ch}} \equiv \Gamma_{\sigma-\sigma} + \Gamma_{\sigma\sigma}, \quad (18)$$

the charge/spin susceptibility must satisfy the sum rules,

$$\begin{aligned} \frac{T}{N} \sum_q \chi_{\text{ch}}(q) &= \frac{T}{N} \sum_q \frac{2\chi_{\text{ph}}(q)}{1 + U_{\text{ch}}\chi_{\text{ph}}(q)} \\ &= n + 2\langle n_{\uparrow}n_{\downarrow} \rangle - n^2, \end{aligned} \quad (19)$$

$$\begin{aligned} \frac{T}{N} \sum_q \chi_{\text{sp}}(q) &= \frac{T}{N} \sum_q \frac{2\chi_{\text{ph}}(q)}{1 - U_{\text{sp}}\chi_{\text{ph}}(q)} \\ &= n - 2\langle n_{\uparrow}n_{\downarrow} \rangle. \end{aligned} \quad (20)$$

The RPA-like form of the susceptibilities can be readily derived if we assume that the irreducible four-point vertices  $\Gamma$ 's are local in time and space. Since the self energy corresponding to the trial Luttinger-Ward functional is constant, the irreducible susceptibility  $\chi_{\text{ph}}$  coincides with the non-interacting form. As a first step in the approximation for the chemical potential  $\mu$ , we choose the same value as that of the non-interacting system,  $\mu_0$ .

The equations (19) and (20) determine  $U_{\text{sp}}$  and  $U_{\text{ch}}$  as a function of the double occupancy,  $\langle n_{\uparrow}n_{\downarrow} \rangle$ . If we follow the idea of the local-field approximation for the electron gas due to Singwi *et al.*,<sup>41)</sup> we can assume a relation,

$$U_{\text{sp}} \equiv g_{\uparrow\downarrow}(0)U, \quad (21)$$

$$g_{\uparrow\downarrow}(0) \equiv \frac{\langle n_{\uparrow}n_{\downarrow} \rangle}{\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle}. \quad (22)$$

from which  $U_{\text{sp}}$  or  $U_{\text{ch}}$  can be determined self-consistently.

In the next level of the approximation, the self energy is assumed to be

$$\begin{aligned} \Sigma_{\sigma}^{(1)}(k) &= U n_{-\sigma} + \frac{U}{2} \frac{T}{N} \\ &\times \sum_q [U_{\text{sp}}\chi_{\text{sp}}(q) + U_{\text{ch}}\chi_{\text{ch}}(q)] G_{\sigma}^{(0)}(k+q) \end{aligned} \quad (23)$$

for which Green's function is given as

$$G_{\sigma}^{(1)}(k) = \frac{1}{i\omega_n + \mu_1 - \varepsilon_{\mathbf{k}}^0 - \Sigma_{\sigma}^{(1)}(k)}, \quad (24)$$

where  $\mu_1$  is obtained by the condition,

$$n = \frac{T}{N} \sum_k G_{\sigma}^{(1)}(k) \exp(-i\omega_n 0^-).$$

An important advantage of this expression for the self energy is that it satisfies the relation,  $\text{Tr}\Sigma^{(1)}G^{(0)} = 2U\langle n_{\uparrow}n_{\downarrow} \rangle$ . We can then use the extent to which this relation is numerically fulfilled as an internal accuracy check. Using  $G^{(1)}$ , Vilk *et al.*<sup>33)</sup> succeeded to reproduce the pseudogaps and the Hubbard bands in the 2D Hubbard model on square lattice.

When the Luttinger sum rule,

$$1/N \sum_{\mathbf{k}} \theta(-\varepsilon_{\mathbf{k}} + \mu_1 - \Sigma^{(1)}) = n_{\sigma},$$

is satisfied, we can take the approximation  $\mu_1 - \Sigma(\mathbf{k}_F, 0) = \mu_0$ . Vilk *et al.*<sup>33)</sup> suggests that, if one considers a region near the half-filling or in the strong-coupling regime, one may improve the approximation by using  $\mu_1 - \Sigma(\mathbf{k}_F, 0)$  in place of  $\mu_0$  in calculating the irreducible susceptibility,  $\chi_{\text{ph}}$ .

## §3. Numerical results

### 3.1 FCC lattice

Now we turn to the present numerical results. We first focus on the FCC lattice. We study the following two cases; (i) a finite  $t' = 0.5$  with  $n = 0.2, 0.6, 1.0$  and (ii) nearest-neighbor hopping only ( $t' = 0$ ) for the same set of band fillings. The DOS for the non-interacting case is displayed in Fig. 2(a), which is highly asymmetric and has a peak around the bottom of the band. This is exactly the situation studied by Kanamori<sup>1)</sup> with the T-matrix approximation: a dilute case with a large DOS at the Fermi level.

Fig. 2. The density of non-interacting states for (a) FCC lattice with  $t' = 0$  (solid line) or  $t' = 0.5$  (dashed line), (b) BCC lattice with  $t' = 0$  (solid line) or  $t' = 1.0$  (dashed line), and (c) SC lattice.

In introducing the interaction, we start with a discussion on how strong the Coulomb interaction may be for the FLEX approximation to be reliable. In Fig. 3, we plot the static magnetic susceptibility,  $\chi \equiv \partial \text{Tr}[\sigma_z G]/\partial h$ , and the RPA spin susceptibility,  $\chi_{\text{RPA}}(\mathbf{0}, 0)$ , as a function of temperature  $T$  for  $t' = 0.5$ ,  $n = 0.2$  for various values of  $U = 0.4 \sim 2.0$ . We deliberately took  $t' = 0.5$  and  $n = 0.2$  because the ferromagnetic spin fluctuation turns out to be the strongest for this parameter set as we shall see below, so that FLEX is expected to be least reliable. Indeed, the difference between  $\chi$  and  $\chi_{\text{RPA}}$  is seen to be large for  $U = 2$ . This means that we cannot approximate the irreducible effective interaction or the four-point vertex  $\Gamma = \delta^2\Phi/\delta G\delta G$  as  $U$  in this case.

As a further check, Fig. 4 looks at the double occupancy,  $\langle n_{\uparrow}n_{\downarrow} \rangle$  normalized by  $\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$ , evaluated from the relation,  $\text{Tr}G_{\sigma}\Sigma_{\sigma} = U\langle n_{\uparrow}n_{\downarrow} \rangle$ . We can see that for  $U = 2$  and  $n = 0.2$ ,  $\langle n_{\uparrow}n_{\downarrow} \rangle$  becomes negative, which is unphysical. Hence, for  $t' = 0.5$  and  $n = 0.2$ , a most

Fig. 3. The FLEX static magnetic susceptibility (dashed lines) and the RPA susceptibility (solid lines) for the Hubbard model on an FCC lattice with  $t' = 0.5$  and  $n = 0.2$  as a function of temperature for  $U = 2$ (a),  $U = 1$ (b) and  $U = 0.4$ (c).

stringent case, the FLEX approximation breaks down at least for  $U > 2$ . Thus we set  $U \leq 2$  hereafter.

Fig. 4. A reliability check for the FLEX method from the double occupancy  $\langle n_{\uparrow}n_{\downarrow} \rangle$  normalized by  $\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$  as a function of  $U$  for  $t' = 0.5$  FCC lattice for various values of the band filling,  $n$ .

Now we are in position to present the result for the density of states and susceptibility. Figure 5 shows the DOS for  $t' = 0.5$ ,  $U = 1, 2$  for the density varied from  $n = 0.2$  (a),  $n = 0.6$ (b) to  $n = 1.0$ (c) with  $T = 0.1$ . The Fermi level is seen to be right at the peak of the DOS for  $n = 0.2$ , so that the ferromagnetic state should be favored according to Stoner's mean field picture.

Fig. 5. The density of states (integrated one-particle spectral function) for  $t' = 0.5$  FCC lattice with  $n = 0.2$  (a),  $0.6$ (b),  $1.0$ (c). The solid (dashed) lines are for  $U = 1$ (2). The insets are blow-ups of the DOS around the Fermi level.

If we then look into the RPA FLEX spin susceptibility  $\chi_{\text{RPA}}(\mathbf{k}, 0)$  in Fig. 6, the ferromagnetic spin fluctuation is indeed strong (i.e.,  $\chi(\mathbf{k})$  enhanced at  $\Gamma$  point) for  $n = 0.2$  as expected from the DOS. (Note that the susceptibility takes the same value at  $\Gamma, \mathbf{k} = (0, 0, 0)$  and  $K, (\pi, \pi, \pi)$  for the convention of taking the FCC dispersion (2).)

Fig. 6. The RPA spin susceptibility as a function of the wavenumber over the Brillouin zone (inset) for  $t' = 0.5$  FCC lattice with  $n = 0.2$  (a),  $0.6$ (b) or  $1.0$ (c) for  $U = 0$  (solid lines),  $U = 1$  (dashed lines) or  $U = 2$  (dotted lines).

For an intermediate density  $n = 0.6$ , on the other hand, the ferromagnetic spin fluctuation disappears. This is in contrast with the results by Ulmke,<sup>15)</sup> who predicted, for the strong-coupling regime, that the ferromagnetic state is most favored for intermediate densities, and that there is a finite lower critical density  $n_c = 0.1 \sim 0.2$  below which the ferromagnetic state is not realized. For  $n = 1.0$  (half filling), we cannot find any instabilities at  $(\pi, 0, 0)$  either, which has been predicted by Ulmke in the strong-coupling regime.<sup>15)</sup>

In Fig. 7, we show  $\chi_{\text{RPA}}(0, 0)$  for  $U = 2$  as a function of  $n$ . We can see that the ferromagnetic fluctuation is most dominant for  $n = 0.2 \sim 0.3$ . If we calculate, for  $U = 5$ , the temperature at which  $\chi_{\text{RPA}}(0, 0)$  diverges as a function of the density  $n$ , we find that the temperature takes its maximum value  $\sim 0.1t$  for  $n \sim 0.2$ . Since the value of  $U = 5$  is too large for the FLEX approximation

to be valid, at least for  $n \sim 0.2$  as mentioned above, we cannot naively identify these as the transition temperatures to a ferromagnetic state. However, the density dependence of these temperatures suggests that the ferromagnetic spin fluctuation is most dominant around  $n \sim 0.2$ . Therefore, we believe that the tendency of the ferromagnetic spin fluctuation being most dominant around  $n \sim 0.2$  in the weak coupling regime should be real.

Fig. 7.  $\chi_{\text{RPA}}(0)$  plotted as a function of  $n$  for  $U = 2$  and  $T = 0.1$ .

Having identified in FLEX that the ferromagnetic spin fluctuation is the strongest for FCC with  $n \sim 0.2$ , we move on to check whether the strong ferromagnetic spin fluctuation remains in the TPSC approximation, which includes vertex corrections. The qualitative features of the spin susceptibility  $\chi$  obtained with TPSC has turned out to be similar to  $\chi_{\text{RPA}}$  obtained with FLEX. Here, we focus on how strong the ferromagnetic spin fluctuation diverges for the case of  $n = 0.2$  and  $t' = 0.5$ . We have checked the internal self accuracy, i.e., the difference between  $\text{Tr}\Sigma^{(1)}G^{(1)}$  and  $\text{Tr}\Sigma^{(1)}G^{(0)}$ ,<sup>33)</sup> to find around 10% accuracy at worst. To check the convergence of eq. (19) or eq. (20), 8192 Matsubara frequencies are required, so we have calculated up to  $N = 16^3$ .

The TPSC result for  $1/\chi$  as a function of  $T$  is plotted in Fig. 8 for  $U = 1 \sim 3$ . Here the chemical potential  $\mu$  is approximated to  $\mu_0$ . The result exhibits a Curie-Weiss like behavior ( $\chi \sim 1/(T + \theta)$ ) with  $\theta > 0$  for  $U \leq 3$ , so that the ferromagnetic transition does not take place as far as this result is concerned. If we approximate the chemical potential  $\mu$  as  $\mu_1 - \Sigma(\mathbf{k}_F, 0)$ , as mentioned at the bottom of §IIC, we can see that the ferromagnetic spin fluctuation becomes more divergent ( $\theta < 0$  for  $U = 3$ ) as seen in the inset. For  $t' = 0.5$  and  $n = 0.2$ , a small change in the chemical potential causes large changes in the solution for  $U_{\text{sp}}$  or  $U_{\text{ch}}$  (eqns(19,20)). However, the tendency detected here that the chemical potential decreases as the approximation for the chemical potential is improved should be correct, and it can be shown, at least in the present case of FCC, that  $U_{\text{sp}}$  becomes larger for smaller  $\mu$ . Therefore, although  $\mu = \mu_1 - \Sigma(\mathbf{k}_F, 0)$  suffers from some numerical inaccuracies due to an error in the Padé fit to  $\Sigma(\mathbf{k}_F, 0)$ , the dominance of the ferromagnetic spin fluctuation should be reliable.

Fig. 8. The inverse of spin susceptibility for FCC in the TPSC approximation as a function of  $T$  for  $U = 1$ (□),  $U = 2$ (+) or  $U = 3$ (×), where  $\mu_0$  is adopted for the chemical potential. The inset is a similar plot, where  $\mu_1 - \Sigma(\mathbf{k}_F, 0)$  is adopted for the chemical potential.

When we turn off the next nearest neighbor hopping ( $t' = 0$ ), the DOS's obtained by FLEX for  $n = 0.2$ (a),  $n = 0.6$ (b), and  $n = 1.0$ (c) in Fig. 9 show that the peak around the bottom becomes much weaker than that for

$t' \neq 0$ . Accordingly,  $\chi_{\text{RPA}}(\mathbf{k}, 0)$  obtained with FLEX in Fig. 10 shows that the ferromagnetic spin fluctuation at low density ( $n \sim 0.2$ ) is much weaker than that for  $t' = 0.5$ . We can in fact quantify this from the fact that only when  $U$  is taken to be as large as 10 (where FLEX is not reliable) does  $1/\chi_{\text{RPA}}(\mathbf{0}, 0)$  become zero for  $t' = 0$ .

Fig. 9. The density of states for  $t' = 0$  FCC lattice with  $n = 0.2$  (a), 0.6(b), 1.0(c). The solid (dashed) lines are for  $U = 1(2)$ . The insets are blow-ups of the DOS around the Fermi level.

Fig. 10. The RPA spin susceptibility as a function of the wavenumber for  $t' = 0$  FCC lattice with  $n = 0.2$  (a), 0.6(b) or 1.0(c) for  $U = 0$  (solid lines),  $U = 1$  (dashed lines) or  $U = 2$  (dotted lines).

### 3.2 BCC lattice

We next turn to the BCC lattice, a typical bipartite lattice. We again study the two cases in the presence and absence of the next nearest neighbor hopping,  $t'$ ; (i) a finite  $t' = 1.0$  with  $n = 0.3, 0.7, 1.0$ , and (ii) nearest neighbor hopping only ( $t' = 0.0$ ) with  $n = 0.2, 0.6, 0.8, 1.0$ . We set  $T = 0.1$  as before. First, the non-interacting DOS, displayed in Fig. 2(b), has a peak around the band center, which resides exactly at the center for  $t' = 0.0$ , since a bipartite lattice has an electron-hole symmetry when electrons hop to nearest neighbors only. As for the accuracy check,  $\langle n_{\uparrow} n_{\downarrow} \rangle / \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$  remains positive for  $U \leq 2$  for cases (i) and (ii).

We start with the result for a finite  $t' = 1.0$ . If we look at the DOS for  $n = 0.3$ (a),  $n = 0.7$ (b), and  $n = 1.0$ (c) in Fig. 11, for  $n \sim 0.7$  the Fermi level is located around the peak of the DOS, although a fictitious dip appears due to a numerical inaccuracy in the analytic continuation.

Fig. 11. The density of states for  $t' = 1.0$  BCC lattice with  $n = 0.3$  (a), 0.7(b), 1.0(c). The solid (dashed) lines are for  $U = 1(2)$ . The insets are blow-ups of the DOS around the Fermi level.

In Fig. 12, we plot  $\chi_{\text{RPA}}$  obtained with FLEX for  $n = 0.3$ (a),  $n = 0.7$ (b), and  $n = 1.0$ (c). Although a finite size effect (slight wiggles) is visible even when we take  $N = 32^3$ , we believe that the overall feature of the spin structure is reliable. As expected, the ferromagnetic spin fluctuation is dominant when  $E_F$  resides at the peak for  $n \sim 0.7$ , but the enhancement in  $\chi$  is much weaker than that for the FCC lattice with  $t' = 0.5$  and  $n = 0.2$ .<sup>42)</sup> In fact  $1/\chi_{\text{RPA}}(\mathbf{0}, 0)$  does not become zero for any value of  $U$  for  $T = 0.1$ . Although the divergence of the peak in the DOS is as sharp as that of FCC with  $t' = 0.5$ , the strength of the ferromagnetic spin fluctuation differs between these cases. This implies that the peak of the DOS located around the bottom is more advantageous

for the ferromagnetic spin fluctuation than when located around the center.

Fig. 12. The RPA spin susceptibility as a function of the wavenumber for  $t' = 1$  BCC lattice with  $n = 0.3$  (a), 0.7(b) or 1.0(c) for  $U = 0$  (solid lines),  $U = 1$  (dashed lines) or  $U = 2$  (dotted lines).

When we turn off  $t'$  in the BCC lattice, the Fermi level coincides with the peak of the DOS for  $n = 1.0$  as shown in Fig. 13. Here again, the analytical continuation with the Padé approximation is unstable for  $n \geq 0.6$ , causing a dip to appear in the DOS. In Fig. 14, we plot the  $\chi_{\text{RPA}}$  obtained with FLEX for  $n = 0.2 \sim 1.0$ . This time the spin fluctuation becomes dominant at the antiferromagnetic point (X point with  $\mathbf{k} = (\pi, \pi, \pi)$ ) for  $n = 0.8$  and  $n = 1.0$ . For  $n = 1.0$ ,  $1/\chi_{\text{RPA}}(\mathbf{0}, 0)$  becomes zero for  $U \sim 2$  and  $T = 0.1$ . As we shall see below, the antiferromagnetic fluctuation is much stronger than that for the simple cubic lattice.

Fig. 13. The density of states for  $t' = 0$  BCC lattice with  $n = 0.2$  (a), 0.6(b), 0.8(c) or 1.0(d). The solid (dashed) lines are for  $U = 1(2)$ .

Fig. 14. The RPA spin susceptibility as a function of the wavenumber for  $t' = 0$  BCC lattice with  $n = 0.2$  (a), 0.6(b), 0.8(c) or 1.0(d) for  $U = 0$  (solid lines),  $U = 1$  (dashed lines) or  $U = 2$  (dotted lines).

### 3.3 Simple cubic lattice

We finally turn to the SC lattice. We plot the DOS in Fig. 15 for  $n = 0.2$ ,  $n = 0.6$ ,  $n = 1.0$ , while the DOS for the non-interacting case is shown in Fig. 2(c). They are electron-hole symmetric since SC lattice is bipartite. We set  $T = 0.1$ . Here again  $\langle n_{\uparrow} n_{\downarrow} \rangle / \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$  remains positive for  $U \leq 2$ . If we look at  $\chi_{\text{RPA}}$  obtained with FLEX in Fig. 16, the ferromagnetic fluctuation is seen to be suppressed. The only enhancement appears for  $n = 1.0$  at the antiferromagnetic point (K point), but the fluctuation is weaker than that for the BCC lattice above.

Fig. 15. The density of states for  $t' = 0$  SC lattice with  $n = 0.2$  (a), 0.6(b), or 1.0(c). The solid (dashed) lines are for  $U = 1(2)$ .

## §4. Discussions and Summary

We have studied the Hubbard model on 3D FCC, BCC, and SC lattices with the FLEX and the TPSC approximations in a weak-coupling regime. We have cal-

Fig. 16. The RPA spin susceptibility as a function of the wavenumber for  $t' = 0$  SC lattice with  $n = 0.2$  (a),  $0.6$  (b) or  $1.0$  (c) for  $U = 0$  (solid lines),  $U = 1$  (dashed lines) or  $U = 2$  (dotted lines).

culated the spin susceptibility as well as the density of states (integrated single-particle spectral function). For cases in which the DOS is divergent near the bottom of the band and the Fermi level is located around the divergence, the *ferromagnetic* instability is found to be dominant. Such a situation is realized for a low band filling in the FCC lattice with a finite next-nearest neighbor hopping ( $t'$ ) or close to the half-filling in the BCC lattice with a finite  $t'$ . For bipartite lattices (SC and BCC lattices with nearest neighbor hopping only), by contrast, the *antiferromagnetic* fluctuation is dominant around the half-filling.

We have found, among the cases studied, that the strongest ferromagnetic fluctuation occurs for a low band filling FCC lattice with  $t'$ , whose DOS is characterized by the sharpest divergence that resides around the band bottom. From a view of “frustration” we may say the following. In the absence of  $t'$ , FCC is frustrated in that its constituent plaquette is a tetrahedron where antiferromagnetic correlations have to interfere, while BCC is bipartite compatible with antiferromagnetism. Thus they have different situations, before  $t'$  is turned on to make the DOS for BCC divergent. While both of the divergent DOS and the frustration can favor ferromagnetism intuitively, we cannot at present stage distinguish effects of the two. We can still observe that the present result for a stronger ferromagnetic fluctuation in FCC than in BCC implies that the peak of the DOS lying around the bottom of the band may be a key factor. As stressed in Introduction, such a comparison could not have been performed from Kanamori’s theory, which focuses on dilute cases. For ground state, Hanisch *et al.*<sup>20</sup> suggested that the fully-polarized ground state is favored when the DOS diverges near the bottom of the band. On the other hand, we have discussed here the tendency toward ferromagnetic instabilities at the finite temperatures, which includes the possibilities of not only fully-polarized state but also partially polarized state. Hence the relation between the results of Hanisch *et al.* and our results is not trivial and is an interesting future problem.

The discussion on the position of the divergence in DOS and frustration reminds us of a situation in 1D, in a quite different context. In the flat-band ferromagnetism mentioned in Introduction, we can consider quasi-one-dimensional systems in which flat bands are realized. There, flat bands can arise in non-frustrated models (such as a chain of squares),<sup>43</sup> but the flat band resides in the middle of the band, so that the ferromagnetism is shown to be destroyed when  $U$  becomes too large. In frustrated models (such as a chain of triangles), by contrast, the flat band is situated at the bottom, and the ferromagnetism is guaranteed for  $0 < U < \infty$  from the Mielke-Tasaki theorem. Although this observation concerns quite a distinct class of systems, further discussions

may prove fruitful.

The FLEX result for the FCC lattice indeed shows that the ferromagnetic instability is most dominant in the low-density region. This reminds us that Ni has an FCC structure with a low hole concentration on the one hand. On the other, the result is contrasted with a DMFT result for the strong-coupling regime by Ulmke,<sup>15</sup> which suggests that for FCC lattice with  $t' \neq 0$ , the ferromagnetic region only appears above  $n_c = 0.1 \sim 0.2$  and is peaked at an intermediate density ( $n \sim 0.6$ ). It is an interesting future problem to explore how these two regimes are interpolated.

The antiferromagnetic fluctuation, by contrast, appears for bipartite (i.e., electron-hole symmetric) lattices (BCC or SC), and the fluctuation is the strongest for the half-filled BCC with a divergent DOS at the Fermi level (for  $t' = 0$ ) of all the situations surveyed here. We note that it is stronger than that in the half-filled SC lattice whose DOS has only a finite peak. This cannot be understood from  $\chi_{\text{ph}}(\pi, \pi, \pi)$  for non-interacting electrons, since there is not much difference in this quantity between the two cases.

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